

Diethyl butanedioate
123-25-1 | DTXSID2038732

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 216 °C

Global applicability domain: Inside

Local applicability domain index: 1.00

Confidence level: 8.52e-01

Nearest Neighbors from the Training Set

Image not found

Diethyl butanedioate

Measured: 218

Predicted: 216

Image not found

Dipropyl oxalate

Measured: 211

Predicted: 216

Image not found

Propanedioic acid, methyl-, diethyl ester

Measured: 201

Predicted: 205